

Phase of the quantum oscillator

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Requirements of a conjugate operator are emphasized, especially in its role in uncertainty relations. It is argued that in many contexts it is necessary to extend the Hilbert space in order to define a conjugate operator as in gauge theories. Example of a particle in a box is analysed. This is closely related to the quantum oscillator through cosine states of Susskind and Glogower. It is used to justify London's phase wave functions albeit as part of a larger Hilbert space. A new definition phase uncertainty necessitated by periodicity is proposed. It is close to the usual r.m.s. definition. Corresponding number-phase uncertainty relation is obtained and its implications are discussed. Hilbert space of an oscillator is identified with the Hilbert space of a planar rotor with a Z_2 gauge invariance. This is used to construct states analogous to the cosine and sine states and to illustrate unitary equivalence of Hilbert spaces.

I. INTRODUCTION

There is a long history [1–4] for attempts to define phase operator for quantum oscillator and related systems. This is important for quantum optics [3] at both theoretical and experimental levels. We take a new look at this problem here. We argue that in many contexts it is necessary to extend the Hilbert space in order to accommodate the conjugate operator as is done in gauge theories. We use the close relation between a particle in a box and an oscillator provided by the cosine states of Susskind and Glogower [5] to justify London's phase wave functions albeit as part of a larger Hilbert space. This provides a very simple description of the oscillator states. Our strategy allows us to obtain the number-phase uncertainty relation. We introduce a new measure of uncertainty necessitated by periodicity. There are points of contact with many earlier works, especially Refs. [5–10]. However our approach and results are different.

The paper is organized as follows. In sec. II we define a new measure of uncertainty of angular position and obtain uncertainty relation in case of the planar rotor. This is directly related to the corresponding issues for a quantum oscillator. In sec. III, we point out the close relation between a particle in a box and an oscillator provided by the cosine states of Susskind and Glogower [5]. This is very useful to understand the conceptual issues and to resolve them. Therefore we analyse a particle in a box as regards the conjugate momentum operator and uncertainty principle in sec. IV. This shows that when the spectrum of an operator is bounded it is necessary to extend the Hilbert space to accommodate the conjugate

operator and to obtain the expected consequences of Heisenberg uncertainty. We use these results to set the requirements of the conjugate operator in sec. V. The crucial requirement is that the inner product of the eigenstates of the conjugate pair has to be a pure phase upto a constant normalization. Sometimes It is necessary to enlarge the Hilbert space to realize this. This is a standard procedure used in gauge theories as emphasised in sec. VI. We finally obtain the phase wave functions of an oscillator and point out the simplicity they provide in sec. VII. We discuss the number - phase uncertainty relation and its implications in different contexts in sec. VIII. In sec. IX we point out that the Hilbert space of an oscillator can be regarded as that of a planar rotor with a Z_2 gauge invariance. We use this to construct states similar to the sine and cosine states [5] and illustrate the unitary equivalence of Hilbert spaces. In particular the oscillator states can also be represented by a particle in a box with antinodes at the walls. In sec. X we summarize our results. In Appendix A we consider some of the identities used. In Appendix B we discuss the definition of phase operator.

II. THE PLANAR ROTOR

We first consider definition of uncertainty in angular position and the uncertainty relation for a quantum planar rotor. These are directly relevant for the oscillator as discussed in later sections.

Angular momentum basis for a planar rotor is $|n\rangle$, $n = 0, \pm 1, \pm 2, \pm 3, \dots$. There is no problem in defining the phase eigenstates here. They are,

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{-in\theta} |n\rangle \quad (1)$$

and represents the state in which the angular position on the circle is specified with certainty. $|\theta\rangle$ and $|\theta + 2N\pi\rangle$ represent the same state so that the range of θ may be restricted to $[-\pi, \pi)$. Planar angular momentum basis is normalizable, $\langle m | n \rangle = \delta_{mn}$, whereas the phase basis $|\theta\rangle$ is not. $|\theta\rangle$ is not even a well defined state of the Hilbert space. For example, the expansion coefficients in Eqn. 1 are not falling off with n . In a sense, $|\theta\rangle$'s are limit points of vectors of the Hilbert space. Dirac has taught us how to handle this profitably. Orthonormality condition is now replaced by, $\langle \theta | \phi \rangle = \delta^P(\theta - \phi)$ where the periodic Dirac delta function is

$$\delta^P(\theta - \phi) = \sum_{-\infty}^{+\infty} \exp(-in(\theta - \phi)) \quad (2)$$

An abstract state $|\Psi\rangle$ may be completely specified through the wave function $\Psi(\theta) = \langle \theta | \Psi \rangle$. Allowed wave functions are given by normalizable and periodic functions of θ . The inner product is,

$$\langle \Psi | \Phi \rangle = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \Psi^*(\theta) \Phi(\theta) \quad (3)$$

Planar angular momentum operator \hat{L} has the representation $-i\hbar d/d\theta$ when acting on these wave functions as we would expect of a conjugate operator. Thus the phase eigenstates can be consistently defined in this problem even though the conjugate variable has a discrete spectrum.

A. A new measure of phase uncertainty

If we choose the period $(-\pi + \alpha, \pi + \alpha)$, the naive definition of uncertainty in phase is

$$\Delta_\alpha^2 \theta = \int_{-\pi+\alpha}^{\pi+\alpha} \frac{d\theta}{2\pi} (\theta - \langle \theta \rangle)^2 |\Psi(\theta)|^2 \quad (4)$$

where

$$\langle \theta \rangle = \int_{-\pi+\alpha}^{\pi+\alpha} \frac{d\theta}{2\pi} \theta |\Psi(\theta)|^2 \quad (5)$$

There are serious problems with this choice, a consequence of the periodicity of the wave functions. It depends on the choice of α , the origin chosen on the circle. Consider a narrow wave packet centered around $\theta = \theta_0$ on the circle and symmetric about it.

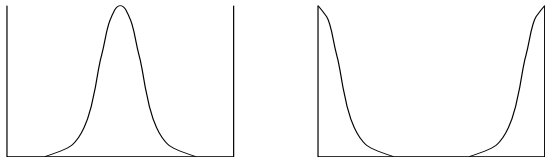


FIG. 1. a. Range chosen such that the wave packet is at the center b. Range chosen such that the wave packet is at the edge

If we choose $\alpha = \theta_0$, (Fig. 1a), we get $\langle \theta \rangle = 0$ as a consequence of symmetry. Then $\theta - \langle \theta \rangle$ is small at the wave packet and we get a small uncertainty in angular position as one would expect for a narrow wave packet. On the other hand if we choose $\alpha = \theta_0 + \pi$, (Fig. 1b), again $\langle \theta \rangle = 0$ due to symmetry. Now $(\theta - \theta_0)^2 \approx \pi^2$ at the wave packet and we get a large uncertainty which is not acceptable. We need a definition which automatically makes the earlier choice.

The usual definition of uncertainty of a variable can be reinterpreted as follows. Consider

$$\int d\theta (\theta - \theta_1)^2 |\Psi(\theta)|^2 \quad (6)$$

which is measuring the mean of square of deviation measured from an arbitrary point θ_1 . This is minimum when $\theta_1 = \langle \theta \rangle$. Thus we are minimizing the mean square of the distance measured from an arbitrary point.

We adopt this principle for our case. Thus our choice is

$$\Delta^2 \theta = \min \int_{-\pi+\alpha}^{\pi+\alpha} \frac{d\theta}{2\pi} (\theta - \langle \theta \rangle)^2 |\Psi(\theta)|^2 \quad (7)$$

where we now minimize w.r.t the parameter α which could be over the entire range $(-\infty, \infty)$. Extremization gives

$$0 = 2(\alpha - \langle \theta \rangle) |\Psi(\pi + \alpha)|^2 - \int_{-\pi+\alpha}^{\pi+\alpha} \frac{d\theta}{2\pi} 2(\theta - \langle \theta \rangle) \frac{d\langle \theta \rangle}{d\alpha} |\Psi(\theta)|^2 \quad (8)$$

noting that $\langle \theta \rangle$, Eqn. 5, itself is a function of α . We have $d\langle \theta \rangle / d\alpha = |\Psi(\pi + \alpha)|^2$ so that the second term is zero. Therefore Eqn. 8 gives the extremization condition to be $\langle \theta \rangle = \alpha$. This simply means that we must choose the range such that the mean value of θ is at the center of that range. There can be many local extrema and therefore many choices of the range satisfying this condition. Some of them could correspond to local maxima also. The second derivative w.r.t α is

$$2(1 - \frac{d\langle \theta \rangle}{d\alpha}) |\Psi(\pi + \alpha)|^2 + 2(\alpha - \langle \theta \rangle) \frac{d^2 \langle \theta \rangle}{d\alpha^2} |\Psi(\pi + \alpha)|^2 \quad (9)$$

The second term is zero at the extrema. Thus the condition for minima is $|\Psi(\pi + \alpha)|^2 < 1$ i.e. the wave function at the edge of the interval should have a magnitude less than one. This is realized in Fig. 1a. On the other hand if the magnitude is greater than one as in Fig. 1b we get a local maxima. In principle there could be more than one minimum and we must choose the absolute minimum.

It is illustrative to present formula for the phase uncertainty in the momentum basis. If $\Psi(\theta) = \sum c_l \exp(il\theta)$ with normalization condition $\sum |c_l|^2 = 1$, then

$$\begin{aligned} \langle \theta \rangle &= \alpha + \sum_{l, L \neq l} c_l^* c_L \frac{(-1)^{l-L}}{-i(l-L)} e^{-i(l-L)\alpha} \\ \langle \theta^2 \rangle &= \frac{\pi^2}{3} - \alpha^2 + 2\alpha \langle \theta \rangle \\ &\quad + 2 \sum_{l, L \neq l} c_l^* c_L \frac{(-1)^{l-L}}{(l-L)^2} e^{-i(l-L)\alpha} \end{aligned} \quad (10)$$

Thus the extremization condition $\langle \theta \rangle = \alpha$ is

$$0 = \sum_{l, L \neq l} |c_l| c_L \left| \frac{(-1)^{l-L}}{(l-L)} \sin((l-L)\alpha - \beta_l + \beta_L) \right| \quad (11)$$

where $c_l = |c_l| \exp(-i\beta_l)$. At these extrema,

$$\Delta_\alpha^2 \theta = \frac{\pi^2}{3} + \sum_{l, L \neq l} |c_l| c_L \left| \frac{2(-1)^{l-L}}{(l-L)^2} \cos((l-L)\alpha - \beta_l + \beta_L) \right|$$

The condition for minimization is $\sum_{l, L \neq l} (-1)^{l-L} |c_l| c_L \cos((l-L)\alpha - \beta_l + \beta_L) \leq 0$. Note that r.h.s of Eqn. 12 is a periodic function of α , and minimization condition simply corresponds to the minimum of this function. Further this minimum is necessarily less than $\pi^2/3$. This is because the cosines all have non-zero Fourier modes so the the mean value of $\Delta_\alpha^2 \theta$ is $\pi^2/3$.

Our definition of the phase uncertainty satisfies all intuitive requirements. It also leads to a simple uncertainty principle of the Heisenberg type as seen below.

B. Uncertainty relation

In an angular momentum eigenstate, the angular position probability is uniformly spread over the entire circle. This is as expected of the conjugate operator. However the way this comes about is somewhat novel.

The uncertainty relation can be worked out in the in the usual way by starting with the inequality $||(\bar{L} + ir\bar{\theta})\Psi|| \geq 0$ where r is a parameter to be varied to get the best inequality. Here $\bar{X} \equiv \hat{X} - \langle \hat{X} \rangle$ for any operator \hat{X} . To begin with we will choose an arbitrary range. Note that, in general, $\theta\Psi(\theta)$ has unequal values at the boundary of the interval even though $\Psi(\theta)$ is periodic. As a consequence the boundary contribution

$$\int_{-\pi+\alpha}^{\pi+\alpha} \frac{d\theta}{2\pi} \frac{d}{d\theta} (\theta |\Psi(\theta)|^2) \quad (13)$$

is not zero but $|\Psi(\pi+\alpha)|^2$. This gives a new contribution to the uncertainty relation:

$$\Delta L \Delta_\alpha \theta \geq \frac{\hbar}{2} (1 - |\Psi(\pi+\alpha)|^2) \quad (14)$$

This relation can be derived directly from operator techniques (B). Note that if the range chosen is such that the wave function $\Psi(\pi+\alpha)$ at the edge has magnitude larger than one then the r.h.s. is $|\Psi(\pi+\alpha)|^2 - 1$. This can be arbitrarily large. Also it can become arbitrarily close to zero.

Finally by considering this at the value $\alpha = \alpha_0$ which minimizes $\Delta_\alpha \theta$ we get the uncertainty relation between fluctuations in phase and planar angular momentum:

$$\Delta L \Delta \theta \geq \frac{\hbar}{2} (1 - |\Psi(\pi+\alpha_0)|^2) \quad (15)$$

Note that in this case we are assured that $|\Psi(\pi+\alpha_0)| \leq 1$.

Now we consider various implications of this equation.

i. As the spectrum of \hat{L} is discrete, we can now have a normalizable state $\exp(iL\theta)$ with $\Delta L = 0$. In absence of the extra term on the r.h.s., Eqn. 14, $\Delta \theta$ would then be unbounded. This is not possible because the range of θ is finite. This contradiction is avoided because of the novel form of the r.h.s. For the angular momentum eigenstate, $\Delta L = 0$ and $|\Psi(\theta)| = 1$, so that both sides of Eqn. 14 are zero. The uncertainty in phase is $\pi/\sqrt{3}$ as expected for a random phase distribution [14]. Indeed this is the maximum value of phase uncertainty with our definition. We may see this as follows. We may expect large phase uncertainty for two identical wave packets that are diametrically opposite on the circle. In this case θ has to be measured from the midpoint of the two on the circle. Of the two midpoints, we have to choose the one for which the distance is shorter. Thus the phase uncertainty is made larger by choosing the wave packets to be symmetric about the diametrically opposite points. Consider such normalized wave packets of width δ : $|\Psi(\theta)|^2 = \pi/\delta$ for $\theta \in (\pi/2 - \delta/2, \pi/2 + \delta/2)$ and $(-\pi/2 - \delta/2, -\pi/2 + \delta/2)$. The maximum value of δ is π which corresponds to a uniform probability over the entire circle. We have $\Delta^2 \theta = \pi^2/4 + \delta^2/12$. This is maximized for $\delta = \pi$, i.e. for a uniform probability and the maximum value is $\pi^2/3$.

ii. We now consider how the inequality is satisfied for a narrow normalized wave packet

$$\Psi(\theta) = \sqrt{\tanh \epsilon} \sum_{-\infty}^{\infty} e^{-|l| \epsilon + i l (\theta - \beta)} \quad (16)$$

which becomes the periodic delta function at $\theta = \beta$ in the limit $\epsilon \rightarrow 0$ (Appendix A). Now

$$\Psi(\theta) = \sqrt{\frac{(1 - e^{-2\epsilon})^3}{(1 + e^{-2\epsilon})}} \frac{1}{(1 - e^{-\epsilon})^2 + 4 \sin^2((\theta - \beta)/2)} \quad (17)$$

This is a wave packet of scale $O(\epsilon)$. Since it is peaked symmetrically about $\theta = \beta$, we must choose the range $(-\pi + \beta, \pi + \beta)$ for calculating uncertainty in θ according to our prescription, Eqn 7. For small ϵ we get by a rescaling $\theta = x\epsilon$,

$$\Delta^2 \theta = 4\epsilon^2 \int_{-\infty}^{\infty} \frac{dx}{2\pi} \frac{x^2}{(1 + x^2)^2} + O(\epsilon^3) \quad (18)$$

so that $\Delta \theta = \epsilon + O(\epsilon^2)$ as one would expect for a wave packet of width ϵ . Thus the phase uncertainty can be made arbitrarily small. Since $\langle L \rangle = 0$, we have $\Delta L = \langle L^2 \rangle$ and $\Delta L = \sqrt{2} \hbar (e^\epsilon - e^{-\epsilon})^{-1}$. Therefore $\Delta L = \hbar / (\sqrt{2} \epsilon + O(\epsilon))$ diverges as $1/\epsilon$ as for a wave packet of size ϵ in position space. We have $\Delta L \Delta \theta = \hbar / \sqrt{2} + O(\epsilon)$. This satisfies the uncertainty relation Eqn. 15 because the wave function at the edge of the interval $\Psi(\beta + \pi) = O(\sqrt{\epsilon^3})$ is very small.

iii. We now consider a normalized state

$$\Psi(\theta) = \cos\gamma e^{i\theta} + \sin\gamma e^{-i\beta} e^{iL\theta} \quad (19)$$

for $l \neq L$. For small γ this is dominated by the angular momentum state l with a small admixture of angular momentum L . The extremization condition gives $\sin((l-L)\alpha + \beta) = 0$. We get $\Delta^2\theta = \pi^2/3 - 2(l-L)^{-2}|\sin(2\alpha)|$. On the other hand, $\Delta L = |(l-L)\sin(2\alpha)|\hbar/2$. Thus, $\Delta L \Delta\theta = |\sin(2\alpha)|\sqrt{\pi^2(l-L)^2/3 - 2|\sin(2\alpha)|}\hbar/2$. This is always larger than the r.h.s. of our uncertainty relation which is now $|\sin(2\alpha)|\hbar/2$.

III. ANALOGY TO A PARTICLE IN A BOX

In this section we point out that the cosine states of Susskind and Glogower [5] relate the stationary states of an oscillator and a particle in a box. We use this for understanding some conceptual issues regarding the phase operator of an oscillator in the next section.

Eigenstates of the number operator \hat{N} of an oscillator are denoted by $|n\rangle$, $n = 0, 1, 2, \dots$. The label is truncated from below. This is the cause underlying the difficulties in defining the conjugate phase operator. Susskind and Glogower [5] (henceforth to be referred to as SG) constructed eigenstates of the ‘cosine operator’ $\hat{c} = \sum_{n=1}^{\infty} (|n\rangle\langle n-1| + |n-1\rangle\langle n|)$. This operator is self adjoint and has a continuum set of eigenstates (in the generalized sense). We label them $|\theta\rangle$. (We are using a different notation than the usual ket only to distinguish this state from the angular position eigenstate $|\theta\rangle$ defined in the sec.II.) The corresponding eigen value is $\cos\theta$.

$$|\theta\rangle = \sum_{n=0}^{\infty} \sin((n+1)\theta) |n\rangle \quad (20)$$

These states are not well defined states of the Fock space as with the states in Eqn. 1. They have to be handled in the same way as using the Dirac formalism. Being eigenstates of a Hermitian operator they form a complete orthonormal set. The inner product of two such states is, (see Appendix A)

$$\begin{aligned} \langle \theta | \phi \rangle &= \sum_{n=0}^{\infty} 2\sin((n+1)\phi)\sin((n+1)\theta) \\ &= \delta^P(\phi - \theta) - \delta^P(\phi + \theta) \end{aligned} \quad (21)$$

$|\theta\rangle$ is the same as $|\theta + \pi\rangle$ and it suffices to choose the range $[0, \pi)$ for θ . Then the second δ function drops out and we get the Dirac delta function orthonormality.

Instead of $\langle \theta | \Psi \rangle$ we may use the wave function $\langle \theta | \Psi \rangle$ to describe the states of an oscillator. Then the stationary state $|n\rangle$ of an oscillator has the wave function $\sin((n+1)\theta)$. Let us presume that there is an apparatus to measure the cosine operator. Then the stationary

states of an oscillator are exactly those of a particle in a box in the usual Schroedinger description. Thus a reformulation of an oscillator using the cosine operator in place of the position operator maps its eigenstates to that of a particle in a box. (This is discussed further in sec. IX).

IV. SOME CONCEPTUAL ISSUES

In this section we analyse a particle in a box to resolve some conceptual issues regarding the conjugate operator and uncertainty relation.

Consider a particle in a box with the position x in the range $[0, \pi)$. The states of the system are linear combinations of $\sin((n+1)x)$, $n = 0, 1, 2, \dots$. It appears that the momentum operator $-i\hbar d/dx$ is not defined on the Hilbert space. It would take a sine function to a cosine function which is not a state of the Hilbert space. This raises the question as to whether the Heisenberg uncertainty relation can be applied to the system. The text book derivation of the zero point energy of a particle in box uses precisely the Heisenberg uncertainty. A formal way of justifying this is as follows. Enlarge the Hilbert space to one spanned by the plane waves $\exp(\pm inx)$, $n = 1, 2, 3, \dots$. The momentum operator $-i\hbar d/dx$ is well defined on this enlarged Hilbert space. If we include $n = 0$ wavefunction also we get precisely the planar rotor basis, Eqn. 1. We may therefore apply the uncertainty relation Eqn.15. However we use it only for the ‘physical states’ of the particle in a box i.e. those spanned by the sine functions only. In particular this means that the state with $\Delta L = 0$ is not an allowed state.

To obtain uncertainty relation we regard the wave functions of the particle in a box as a subset of wave functions of the planar rotor. $x \in (0, \pi)$ is identified with $\theta \in [-\pi, \pi)$. The wave functions are periodic repetitions of the wave functions of a particle in a box. They vanish at $\theta = \pi \pmod{2\pi}$. The uncertainty in position is defined as in sec. II A. For all ‘physical states’ the probability for angular momenta $\pm L$ are equal. Therefore $\langle \hat{L} \rangle = 0$ and $\Delta^2 L = \langle \hat{L}^2 \rangle$. Now, \hat{L}^2 is a meaningful operator on the physical states, as it takes the sine functions into sine functions. It is precisely the Hamiltonian of the system. Thus the uncertainty relation as obtained by extending the Hilbert space constrains the expectation value of energy and the spread in position. In particular it gives a zero point energy.

The lesson to be learnt from this example is that when the spectrum of an oscillator is bounded, it is necessary to extend the Hilbert space and regard the states of the original Hilbert space as ‘physical states’ of the system. Only then it is possible to define the conjugate operator and obtain implications of the uncertainty relations for the original operator.

V. REQUIREMENTS OF A CONJUGATE OPERATOR

Our discussion of the planar rotor and a particle in a box is to emphasize that the definition of the conjugate operator is more involved when the spectrum of the original operator is discrete or compact. In this section we formally state the properties required of a conjugate operator and the necessity to enlarge the Hilbert space at times to accommodate it.

In case of the planar rotor, angular momentum operator has the traditional form $-i\hbar d/d\theta$ when acting on the wave functions $\Psi(\theta)$. But its commutator with the angular position operator (Appendix B) is not the standard one. Nevertheless expectations of the Heisenberg uncertainty principle are in operation. In the angular position eigenstates $\exp(i l \theta)$, the angular position probability is spread uniformly over all angles as the probability amplitude is just a phase. Consider a normalized wave packet peaked around θ_0 on the circle. In the limit of an infinitely narrow wave packet, it is the periodic delta-function $\delta^P(\theta - \theta_0)$ upto a diverging normalization. The probability amplitude to find angular momentum l is proportional to $\exp(-i l \theta_0)$, Eqn. 2, and hence there is a uniform spread in all angular momenta. Thus in this example the crucial feature of the conjugate operator that is relevant for the Heisenberg uncertainty principle is not the canonical Heisenberg commutation relation. It is the fact that the matrix elements $\langle \theta | l \rangle$ of the eigenstates of conjugate operators are all phase factors upto an overall normalization.

Now consider a particle in a box. A wave packet which is localized around a point x_0 can be expanded in the complete set, the sine functions. In the limit of the wave packet becoming infinitely narrow, we get a representation (upto an infinite normalization) of the position eigenstate for the problem (Appendix A). $\Psi(x) \equiv \sum_0^\infty \sin((n+1)x_0) \sin((n+1)x)$. The probability $\sin^2((n+1)x_0)$ for different n 's are not of same magnitude. But these coefficients refer to an expansion in the eigenstates of the Hamiltonian and not of conjugate momentum operator. To get the eigenstates of the latter we enlarged the Hilbert space in sec.IV. Now in this basis the position eigenfunction has the expansion $\Psi \subset x \supset = \sum_{-\infty}^\infty \exp(inx_0) \exp(-inx)$ as in the planar rotor. Now the coefficients are all phase factors and the probability is spread uniformly over all momenta. Thus again the crucial feature of the conjugate operator is that the matrix element is a phase. We had to enlarge the Hilbert space to accommodate the conjugate operator in this case.

Consider a self adjoint operator \hat{A} with a complete orthonormal set of eigenstates $|\alpha\rangle$ with real eigenvalues α . This may be a continuum set or discrete; of a bounded or unbounded spectrum; or a combination of these. The

conjugate operator \hat{B} is required to have the following properties in order to realize the expectations from the Heisenberg uncertainty principle. i. It is a self adjoint operator with a complete orthonormal set of eigenstates $|\beta\rangle$ with real eigenvalues β . ii. The matrix elements $\langle \beta | \alpha \rangle$ should all be phase factors upto a normalization independent of the labels α or β . The original Hilbert space may not admit an operator with these properties. Then we have to enlarge the Hilbert space and regard the states of the original Hilbert space as 'physical states'. We consider further examples of this in latter sections.

VI. ANALOGY WITH GAUGE THEORIES

In this section we point out that our technique of enlarging the Hilbert space is the standard procedure used in gauge theories. Therefore various techniques of quantization used in gauge theories can be adopted for our systems.

In quantum electrodynamics, to get a Hamiltonian description we are forced to introduce an unphysical operator $A_i(x)$, the vector potential, as the conjugate of $E_i(x)$, the electric field. The gauge invariant operator, magnetic field $B_i(x)$, has more complicated commutation relations with $E_i(x)$. If we are using a Schrodinger wave functional description $\Psi[A_i(x)]$, not all wave functionals are in the physical Hilbert space. Only such which have same values for any given $A_i(x)$ and $A_i(x) + \nabla_i \lambda(x)$ (where the function $\lambda(x)$ is arbitrary) are physical states.

As we are going to use the analogy with quantum electrodynamics, we give a quick review of the various quantization procedures used there. i) We may work with only the subspace of the Hilbert space consisting of physical states, those that satisfy the Gauss law constraint, $\nabla_i E_i(x)|_{phys} = 0$. ii) We may choose a representative from gauge equivalent configurations. A common choice is the Coulomb gauge fixing condition $\nabla_i A_i = 0$. Then arbitrary functionals $\Psi[A_i]$ of such $A_i(x)$ may be used. However the canonical commutation relation may have to be modified to account for the gauge fixing constraint. iii) We may eliminate the redundant degrees altogether, as in the axial gauge where $A_3(x)$ is eliminated and only A_1, A_2 are used. iv) We may use the electric field basis and solve the Gauss law. v) There is also the BRST quantization involving additional Grassmann degrees of freedom.

Each of the above procedures may be adopted for the present situation. They would all give same results though a particular representation may be advantageous for a given purpose. We directly pass on to the most convenient choices for the present case.

VII. PHASE WAVEFUNCTIONS OF THE QUANTUM OSCILLATOR

In sec. V we have argued that the crucial requirement for the conjugate phase description of the number operator eigenstates is that the wave function $\langle \theta | n \rangle$ of the number eigenstate should be phase factors upto a normalization so that it has uniform probability for each value of the phase. Many authors, in particular SG [5], have pointed out problems with this. If we define the phase eigenstates,

$$|\theta\rangle = \sum_0^{\infty} e^{-in\theta} |n\rangle \quad (22)$$

with the sum running over only the non-negative integers, then the states are neither linearly independent nor orthonormal: The inner product is (Appendix A),

$$(\langle \theta | \phi \rangle) = \frac{1}{2} \delta^P(\theta - \phi) + i e^{i(\theta - \phi)/2} \operatorname{cosec}(\theta - \phi)/2 \quad (23)$$

The way out of this problem is suggested by our analogy of a particle in a box. We enlarge the Hilbert space though it is now used in a different way. This Large Hilbert space has the basis $|n\rangle$ where n now takes both positive and negative integral values. The physical states are only those with $n = 0, 1, 2, \dots$. The purpose of having the additional states is to be able to define the conjugate phase operator. The basis of the Large Hilbert space is in 1:1 correspondence with the angular momentum basis of the planar rotor and we may define the conjugate operator $\hat{\theta}$, Eqn. B2, and its eigenstates $|\theta\rangle$, Eqn. 1. These states are free of the problems encountered by SG [5]. The eigenstate $|\theta\rangle$, Eqn. 1, is built out of both positive and negative n states and is therefore not a physical state. But this does not mean that we cannot use it to describe the states of the subspace.

The analogy with the gauge theories is as follows. We may describe the physical states of quantum electrodynamics using the wave functional $\langle \{A_i(x)\} | \Psi \rangle$ even though the gauge potential $\hat{A}_i(x)$ is not an operator on the physical subspace. Only, not all wave functionals are allowed but just those satisfying the Gauss constraint, $\nabla_i \delta \Psi(A) / \delta A_i(x) = 0$. The analogous constraint for us is that the physical states should be composed of only non-negative values of the angular momentum $-i\hbar d/d\theta$. This has some analogy to the Gupta-Bleuler technique in quantum electrodynamics.

As in gauge theories, even though $|\theta\rangle$ is not a physical state, states of the physical Hilbert space may be described via the wave functions $\Psi(\theta) = \langle \theta | \Psi \rangle$ and all observables may be computed from it. For a state with the occupation number expansion $|\Psi\rangle = \sum_0^{\infty} c_n |n\rangle$ the corresponding phase wave function is $\Psi(\theta) = \sum_0^{\infty} c_n \exp(in\theta)$. This is precisely the phase representation of state vectors implicit in papers of London

[15] and often used in quantum optics [16–18]. The major advantage of our point of viewing it as a subspace of the Large Hilbert space is that we can obtain the number - phase uncertainty relation and its implications. This is discussed in the next section. Note that it is not possible to resolve a general wave packet using positive Fourier modes only. (In particular, the δ - function cannot be resolved and we cannot realize the phase eigenstate.) We construct other physical states of narrow phase distribution in the next section.

Working with the Large Hilbert space provides a simplification both conceptually and computationally. The time evolution of a state has a simple form when the phase description is used. $\Psi(\theta) \rightarrow \Psi(\theta - \omega t)$ is obtained by the classical evolution $\theta \rightarrow \theta - \omega t$ as expected. Inner product of any two wave functions $\Psi(\theta)$ and $\Phi(\theta)$ is given by Eqn. 3. The annihilation operator has the simple representation $\hat{a} = e^{-i\theta} \sqrt{-i\hbar/d\theta}$ when acting on the phase wave functions. Note that by itself the multiplication by $e^{-i\theta}$ takes the ground state of the oscillator outside the physical subspace and therefore not a physical operator. But the operator $\sqrt{-i\hbar/d\theta}$ gives zero precisely on this state making \hat{a} a physical operator. Thus the Dirac's decomposition of the annihilation and creation operators is now valid. Using the Large Hilbert space has been crucial for making this possible. The contradiction noticed by Louiselle [13] and SG [5] is not valid now. $\hat{u} = \exp(-i\theta)$ satisfies $\hat{u}\hat{u}^* = \hat{u}^*\hat{u} = 1$ because now it is an operator in the Large Hilbert space.

VIII. NUMBER-PHASE UNCERTAINTY RELATION

We now consider the number-phase uncertainty relations for the quantum oscillator. As the phase wave functions are a subset of the wave functions of a planar rotor we may directly use the uncertainty relation Eqn. 15. But the following points should be kept in mind. We use the uncertainty relation for physical states only, though it is valid for other states also. $\hat{\theta}$ (Appendix B) is not a 'physical' operator. It generates negative Fourier modes also when acting on a physical state. Nevertheless the uncertainty relation Eqn. 15 gives a constraint on the relative spreads in the occupation number distribution (represented by $|c_n|^2$) *vis-a-vis* the phase (represented by $|\Psi(\theta)|^2$). For this purpose the r.m.s. spread in θ , Eqn. 7, is again relevant and meaningful as it stands. We may express this in stronger words as follows: The wave function $\Psi(\theta)$ contains complete information of the abstract state $|\Psi\rangle$ and therefore meaningful even if $|\theta\rangle$ is not a physical state. So long as the states are described by the wave functions $\Psi(\theta)$, $\Delta\theta$ as defined in Eqn. 7 is calculable and therefore a measurable object. Further it is a measure of the spread in θ . Therefore the number -phase

uncertainty relation is given by Eqn 15 with $\Delta L/\hbar$ being interpreted as the r.m.s. spread in the number.

The occupation number eigenstate $|n\rangle$ has a uniform spread in the phase as expected and meets the ‘acid test’ of Barnett and Pegg [14]. On the other hand the phase eigenstate $|\theta\rangle$ is not a physical eigenstate and therefore the discussion concerning it is not relevant for the oscillator.

We now consider states [2,8,20] which are sometimes referred to as coherent phase states: $\Psi_\zeta(\theta) = \sqrt{1-|\zeta|^2} \sum_{n=0}^{\infty} \zeta^n \exp(in\theta)$. These are obtained as eigenstates of the non-Hermitian ‘exponential operator’ $E = \sum_{n=0}^{\infty} |n\rangle\langle n+1|$. This is formally similar to the narrow wave packets of the planar rotor Eqn. 16 with $\zeta \rightarrow \exp(-\epsilon - i\beta)$, but only positive Fourier modes are involved. Therefore it is of interest to see whether they correspond to states of the oscillator with a narrow phase distribution. Note that with $\zeta = \exp(-\epsilon - i\beta)$,

$$\begin{aligned} |\Psi_\zeta(\theta)|^2 &= (1 - e^{-2\epsilon}) \sum_{m,n=0}^{\infty} e^{-(m+n)\epsilon} e^{i(n-m)(\theta-\beta)} \\ &= (1 - e^{-2\epsilon}) \sum_{N=0}^{\infty} e^{-2N\epsilon} \sum_{r=-\infty}^{+\infty} e^{-r\epsilon} e^{ir(\theta-\beta)} \quad (24) \end{aligned}$$

This, ofcourse, has both positive and negative Fourier modes. Moreover it is precisely the wave packet of the planar rotor, Eqn. 16, considered as an approximation to the periodic delta function (Appendix A). For $\epsilon \rightarrow 0$, $\Psi_\zeta(\theta)$ is sharply peaked in θ around $\theta = \beta$. Thus it is a state of narrow phase distribution. It is a complex square root of the Poisson kernel (Appendix A), and in the limit $\zeta \rightarrow 1$ it may be regarded as square root of the periodic delta function.

As the probability density is peaked and symmetric about $\theta = \beta$, we expect that we have to choose $\alpha = \beta$, Eqn. 7, for the uncertainty in phase. Therefore we get

$$\Delta^2(\theta) = (1 - |\zeta|^2) \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \frac{\theta^2}{(1 - |\zeta|^2)^2 + 4|\zeta|^2 \sin^2(\theta/2)} \quad (25)$$

The integral is finite in the limit $|\zeta| \rightarrow 1$ and has the value $\ln 4$. Therefore $\Delta\theta \rightarrow 0$, and we get a vanishingly small uncertainty in phase. On the other hand, $\langle \hat{N} \rangle = \hbar|\zeta|(1 - |\zeta|^2)^{-1}$, $\langle \hat{N}^2 \rangle = \hbar^2|\zeta|(1 + |\zeta|)(1 - |\zeta|)^{-3}$ so that $\Delta N = |\zeta|^2(1 - |\zeta|^2)^{-1}$. Note the following features. As $\epsilon \rightarrow 0$, $\Delta\theta = 2\sqrt{\ln 2}\sqrt{\epsilon} + O(\epsilon)$. Thus the uncertainty in θ is much larger $O(\sqrt{\epsilon})$ than the scale $O(\epsilon)$ of the wave packet, in contrast to the free particle or the wave packet, Eqn. 16, for the planar rotor. The reason is that $\Psi_\zeta(\theta)$ is quite wide. It is however true that we can obtain states of arbitrarily small uncertainty in phase by choosing ϵ arbitrarily small. In this state $\Delta N \sim (2\epsilon)^{-1}$ diverges as is to be expected. The product $\Delta N \Delta\theta \sim 1/\sqrt{\epsilon}$ is much larger than the r.h.s. of the uncertainty relation. Note that $|\Psi(\pi + \beta)|^2$ is vanishingly small in this limit so that

the extra term on the r.h.s. of the uncertainty relation Eqn. 16 has almost no effect.

We now consider the phase uncertainty for coherent state $|z\rangle$ which has the normalized phase wave function

$$\Psi_z(\theta) = e^{-r^2/2} \sum_{n=0}^{\infty} \frac{r^n}{\sqrt{n!}} e^{in(\theta-\beta)} \quad (26)$$

where $z = r \exp(-i\beta)$. This is symmetrically peaked around $\theta = \beta$. Therefore we have to choose the range $(-\pi + \beta, \pi + \beta)$. (This can be checked directly.) The uncertainty in phase $\Delta\theta$ is

$$\begin{aligned} \Delta^2\theta &= \frac{\pi^2}{3} + e^{-r^2} \sum_{m,n \neq m} \frac{2(-r)^{m+n}}{\sqrt{m!n!}(m-n)^2} \\ &= 4e^{-r^2} \sum_{n=0}^{\infty} \frac{r^{2n}}{\sqrt{n!}} \sum_{s=1}^{\infty} \frac{(-r)^s}{s^2} \left(\frac{1}{\sqrt{(n+s)!}} - \frac{1}{\sqrt{n!}} \right) \quad (27) \end{aligned}$$

This is small for large r . This can be directly seen from the form of $|\Psi(\theta)|^2$. The half width is $O(r^{-1})$. On the other hand the spread in the occupation number is $\Delta N = r$. The uncertainty relation is satisfied for all r , though for large r it approaches an equality.

IX. OSCILLATOR AS A PLANAR ROTOR WITH Z_2 GAUGE INVARIANCE

In this section we point out that our adhoc procedure of extending the Hilbert space is related to gauge invariance idea. We use it to construct states analogous to the sine and cosine states of SG [5].

We define a Large Hilbert space \mathcal{H} as that of the planar rotor. We define a gauge transformation,

$$P|n\rangle = |-n\rangle, n = 0, \pm 1, \pm 2, \dots \quad (28)$$

This is the parity transformation. Our previous technique of using only the positive Fourier modes is related to this formalism through a gauge fixing as follows. We choose a representative of each gauge equivalent set of states to describe the physical states. Thus we may choose $|n\rangle$ with $n \geq 0$ only.

In this section we handle the gauge invariance differently. We demand the physical states to be those that are invariant under this transformation. Thus the basis for the physical states is $(|n\rangle + |-n\rangle)/\sqrt{2}$, $n = 1, 2, 3, \dots$ in addition to $|0\rangle$ which is already gauge invariant. This labels the basis for \mathcal{H}/\mathcal{P} . We see that there is an one-to-one correspondence with the basis of the oscillator, $|0\rangle = |0\rangle$, $(|n\rangle + |-n\rangle)/\sqrt{2} = |n\rangle$, $n = 1, 2, 3, \dots$

In the Large Hilbert space we have the phase eigenstate $|\theta\rangle$ as in the planar rotor, Eqn.1. However this is not a gauge invariant state and therefore not physical. From Eqn.1 we see that under the gauge transformation, $P|\theta\rangle = |-\theta\rangle$. The transformation of the

wave function is $P\Psi(\theta) = \Psi(-\theta)$. Therefore even periodic functions of θ are physical states. Thus a basis for the physical states consists of only of the even functions $\sqrt{2} \cos(n\theta)$, $n = 1, 2, \dots$ and 1 for $n = 0$.

As with a particle in a box, sec. III, the operator $\hat{L} = -i\hbar d/d\theta$ is not an operator on the physical states as it takes the cosine into a sine function. Since $P\hat{L}P^{-1} = -\hat{L}$, \hat{L} is not gauge invariant. On the other hand \hat{L}^2 is a gauge invariant operator and therefore well defined on the physical Hilbert space. Since $\hat{L}^2|\pm n\rangle = n^2|\pm n\rangle$, we get $\hat{L}^2|n\rangle = n^2|n\rangle$. On the wave functions $\Psi(\theta)$ this means $(-d^2/d\theta^2)\cos(n\theta) = n^2\cos(n\theta)$, $n = 1, 2, 3, \dots$. Therefore we may define uniquely the square root operator, $\hat{N} = \sqrt{\hat{L}^2}$ which has the action $\hat{N} \cos(n\theta) = n \cos(n\theta)$, $n = 1, 2, 3, \dots$. It is a self adjoint operator. This is the number operator in terms of which the oscillator Hamiltonian is simply $\hat{H} = (\hat{N} + 1/2)\hbar\omega$. In this basis, the stationary states of the quantum oscillator have the form $\sqrt{2} \cos(n\theta)$. The time evolution is $\psi_n(t) = \exp(-i(n + 1/2)\omega t)\sqrt{2} \cos(n\theta)$.

For any physical state the amplitude of the wave function at $|\theta\rangle$ is the same as at $|- \theta\rangle$. This means that it is sufficient to choose the range of θ to be $[0, \pi)$. This may be stated in a different way. The combination $|\theta\rangle = (|\theta\rangle + |- \theta\rangle)/\sqrt{2}$ is gauge invariant and can be therefore expanded in terms of the complete basis of physical states $|n\rangle$,

$$\begin{aligned} |\theta\rangle &= \sum_{-\infty}^{\infty} \frac{1}{\sqrt{2}} (e^{in\theta} + e^{-in\theta}) |n\rangle \\ &= \sqrt{2} (|0\rangle + \sum_1^{\infty} \sqrt{2} \cos(n\theta) |n\rangle) \end{aligned} \quad (29)$$

The state $|\theta\rangle$ is not normalizable, but so is the case of the planar rotor where it is well understood. All operations with this state have well defined meaning in the Large Hilbert space. For example,

$$\begin{aligned} \langle\langle \theta | \theta' \rangle\rangle &= (\langle \theta | + \langle -\theta |)(|\theta\rangle + |- \theta\rangle)/2 \\ &= \delta^P(\theta - \theta') + \delta^P(\theta + \theta') \end{aligned} \quad (30)$$

As the range of θ is $[0, \pi)$ the second Dirac delta function drops out from this equation and we get the conventional orthonormality condition.

A. Alternate representation of the physical states related to the $|\theta\rangle$ basis

The gauge invariant states $|\theta\rangle$ that we constructed from $|\theta\rangle$ were the easiest but not the only ones. We construct another appealing representation. We defined the action of the non-trivial element P of the Z_2 group on the rotor states by $P|n\rangle = |-n\rangle$. We could consider other choices: $P|n\rangle = -|-n\rangle$. One disadvantage with this

is that $P|0\rangle = -|0\rangle$ so that it is impossible to obtain gauge invariant states involving $|0\rangle$. One way out is to consider a modified planar rotor corresponding to an electric charge confined to a circle through which is treading a half unit of magnetic flux [21]. Now the planar angular momentum is $n = \pm 1/2, \pm 3/2, \dots$. We may now choose the group action $P|n\rangle = -|-n\rangle$, $n = \pm 1/2, \pm 3/2, \dots$. Now the basis for gauge invariant states is provided by $|n - 1/2\rangle = (|n\rangle - |-n\rangle)/\sqrt{2}$, $n = 1/2, 3/2, \dots$. In the $|\theta\rangle$ basis we get the gauge invariant orthonormal set,

$$\begin{aligned} |\theta\rangle &= \frac{-i}{\sqrt{2}} (|\theta\rangle - |- \theta\rangle) \\ &= \sum_0^{\infty} \sqrt{2} \sin((n + \frac{1}{2})\theta) |n\rangle \end{aligned} \quad (31)$$

We have,

$$\begin{aligned} \langle \theta | \theta' \rangle &= (\langle \theta | - \langle -\theta |)(|\theta\rangle - |- \theta\rangle)/2 \\ &= \delta^P(\theta - \theta') - \delta^P(\theta + \theta') \end{aligned} \quad (32)$$

Again it is sufficient to restrict $\theta \in [0, \pi)$ and we get the orthonormality. This provides a representation of the stationary states of the oscillator in terms of half integer sine functions.

B. Unitary equivalence of Hilbert spaces

The cosine states of SG [5] give stationary states of the oscillator as those of a particle in a box. On the other hand Eqn. 29 give these wave functions as cosines which do not vanish at the boundary. They correspond to stationary states of a particle in a box with reflecting walls which produce antinodes instead of nodes at the walls. Thus the same system, viz. the oscillator, is being described by such disparate systems. This is yet another instance of the unitary equivalence of all Hilbert spaces. Further examples are the following. In case of our other realization of the Z_2 gauge invariance, Eqn. 31, we are realizing the stationary states using sine functions with half integer Fourier modes. The sine states of SG has alternately sine and cosine functions for even and odd Fourier modes respectively.

The cosine and sine states of SG [5] are the complete set of eigenstates of hermitian cosine and sine operators. This assures that their eigenstates form a complete orthonormal set. In the same way, our states constructed from gauge invariance considerations can also be realized as complete set of eigenstates of certain Hermitian operators. These are the operators for which the corresponding wave functions are the probability amplitudes. Thus the oscillator is being probed using different observables in each case. In each case the eigenvalues form a continuum bounded set. The matrix elements $\langle \theta | n \rangle$ provide a

unitary transformation (in the generalized sense) from the denumerable set $|n\rangle = 0, 1, 2, \dots$ to a continuum set $|\theta\rangle \subset [0, \pi)$ in each case.

X. SUMMARY

There are distinct problems to be first addressed in defining the phase of a quantum oscillator. We used the planar rotor and a particle in a box to help us in resolving these issues. These systems are relevant to the oscillator in a deeper way. We used gauge invariance to relate it to the planar rotor and the cosine states [5] to relate it to a particle in a box. We defined a new measure of phase uncertainty, Eqn. 7. This is closest to the r.m.s. definition without having problems with the periodicity of the wave functions. It also gives an uncertainty relation Eqn. 15 that is of the conventional type with crucial differences that avoids contradictions.

We argued that the crucial feature required of a conjugate variable as regards its role in uncertainty principle is that inner product of the eigenstates of the conjugate pair must be pure phase upto an overall normalization. It may be necessary to extend the Hilbert space to accommodate such an operator. We pointed out that this is a standard procedure adopted in gauge theories. We used this connection to justify London's phase wave functions without running into contradictions.

We considered some examples to illustrate the way our uncertainty relation works. We showed that the so called coherent phase states can be used to obtain arbitrarily narrow phase uncertainty.

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APPENDIX A: SOME IDENTITIES

Many of the series used here, e.g. Eqns. 2, 21 are not uniformly convergent. The ratios of successive coefficients are of unit modulus. Such identities can be justified and interpreted in the sense of generalized functions [22]. Heuristic way of obtaining such identities is by regularizing the sum and then taking the limit as described below.

The periodic delta-function can be obtained as a limit of the Poisson kernel [23, 24] $\delta_\epsilon(\theta)$ in the limit $\epsilon \rightarrow 0$.

$$\delta_\epsilon^P(\theta) = \sum_{n=-\infty}^{+\infty} \exp(-n(\epsilon + i\theta))$$

$$\begin{aligned} &= \frac{1 - e^{-2\epsilon}}{1 + e^{-2\epsilon} - 2e^{-\epsilon}\cos\theta} \\ &\rightarrow 0, \text{ as } \epsilon \rightarrow 0, \text{ if } \theta \neq 0(\text{mod } 2\pi), \\ &\rightarrow \infty, \text{ as } \epsilon \rightarrow 0, \text{ if } \theta = 0(\text{mod } 2\pi) \end{aligned} \quad (\text{A1})$$

as required for the δ function. In particular, $\int d\theta/(2\pi)\delta_\epsilon^P(\theta) = 1$ for all ϵ including the limit $\epsilon = 0$. Thus we get $\sum_0^\infty 2\cos n\theta = \delta^P(\theta) - 1$.

We also need the following sums.

$$\begin{aligned} &\sum_1^\infty \sin n\theta \\ &= \lim_{\epsilon \rightarrow 0} \frac{1}{2i} \left(\frac{1}{1 - e^{-\epsilon + i\theta}} - \frac{1}{1 - e^{-\epsilon - i\theta}} \right) \\ &\rightarrow (1/2)\cot\theta/2, \text{ as } \epsilon \rightarrow 0, \text{ if } \theta \neq 0(\text{mod } 2\pi), \\ &\rightarrow 0, \text{ as } \epsilon \rightarrow 0, \text{ if } \theta = 0(\text{mod } 2\pi) \end{aligned} \quad (\text{A2})$$

Thus there is a discontinuity at $\theta = 0(\text{mod } 2\pi)$, but we may simply take $\sum_1^\infty 2\sin n\theta = \cot(\theta/2)$.

APPENDIX B: PHASE OPERATOR

In sec. II B we obtained the uncertainty relation without explicitly introducing the operator $\hat{\theta}$ for the angular position or its commutation relation with the planar angular momentum. The relation can also be obtained by using these operators. Definition of $\hat{\theta}$ presents some novelty [11, 5, 12]. When acting on the wave function $\Psi(\theta)$, $\hat{\theta}$ has the effect of multiplying it by a periodic repetition of θ in the interval $[-\pi, \pi)$. Therefore the action of $\hat{\theta}$ on a continuous periodic function gives a wave function that is discontinuous at the boundary of this interval. In contrast the angular momentum operator $\hat{L} = -i\hbar d/d\theta$ has no such complications. This has the immediate consequence that the commutation relation has an extra term on the r.h.s.

$$[\hat{L}, \hat{\theta}] = -i\hbar(1 - \delta^P(\hat{\theta} - \pi)) \quad (\text{B1})$$

where the operator δ^P is obtained by using the operator $\hat{\theta}$ in place of θ in Eqn. 2. It is this extra term that avoids a contradiction when we take diagonal matrix elements in the angular momentum basis. We get zero on both sides.

Our definition of the $\hat{\theta}$ operator selects the $\theta = 0$ point as special because our saw tooth wave function is antisymmetric about it. We could equally well choose the operator $\hat{\theta}(\alpha) = \hat{\theta} + \pi - \alpha$ which corresponds to discontinuity at $\theta = \alpha(\text{mod } 2\pi)$. Now the commutation relation is

$$[\hat{L}, \hat{\theta}(\alpha)] = -i\hbar(1 - \delta^P(\hat{\theta} - \alpha)) \quad (\text{B2})$$

Note that $\langle \Psi | \delta^P(\hat{\theta} - \alpha) | \Psi \rangle = |\Psi(\alpha)|^2$. This leads to the inequality Eqn. 14.

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